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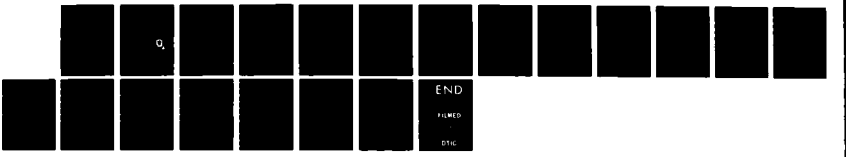

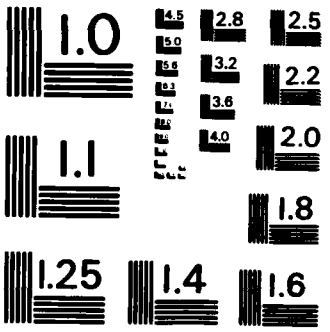

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# Host Materials for Transition-Metal Ions with the $nd^N$ Electronic Configuration

by Clyde A. Morrison
Richard P. Leavitt
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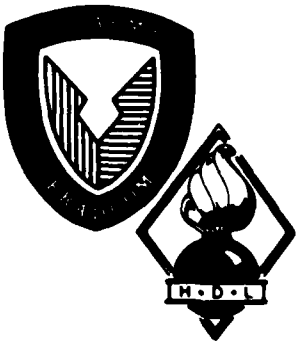

U.S. Army Electronics Research
and Development Command
**Harry Diamond Laboratories**
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Data are given on 12 host materials for lasers that use the transition metal ions. Included in each section are the crystallographic data, x-ray data, lattice sum parameters $A_{\widetilde{nm}}$, crystal field parameters $B_{nm}$(Dq), and spin-orbit constants ($\zeta$). One section contains the phenomenological free ion parameters $F^{(k)}$, $\xi$, and $\alpha$, which have been obtained by fitting the reported free ion data. There is a bibliography for each host which, dependent on that particular host, is more or less complete. The data contained on each host material as well as on new host materials will be added periodically.

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## Contents



## Tables







A1

## 1. INTRODUCTION

The following report contains tables that list information on various potential laser host materials for transition metal ions of the $nd^N$ electronic configuration. Many of the fluorinated host materials were selected from a list supplied by H. P. Jenssen and A. Linz of the Massachusetts Institute of Technology (MIT). We thank them for the use of this list. Also we wish to thank D. Gabbe of MIT for supplying us with a list of fluorinated garnets (almost all the information we have on these garnets was supplied by Gabbe).

A number of host materials were selected because lasers had been reported that used $3d^N$ ions as impurities in those hosts. These host materials, with limited amounts of experimental energy levels, were reported during the early 1960's, and some later work has been done in some of these hosts. Unfortunately, much of the reported absorption data have been taken at room temperature (~300 K) and are quite unreliable because of the presence of vibronics and absorption from excited levels. Further complications arise when the data are extracted from the excitation spectra. There is a real need for low-temperature absorption spectra of many of these ions.

## 2. DISCUSSION OF TABLES

### *2.1 Crystallographic data*

The crystallographic data on each host are given in the notation of the International Tables.[1] The crystallographic data are presented in a short table for each host that lists the following information:

(a) Crystal class, such as triclinic, orthorhombic

(b) Space group symbol and number from the International Tables

(c) Number of chemical formula units, Z, per unit cell

(d) Setting, if there is more than one for that space group in the International Tables

(e) Position (site type in the International Tables), site symmetry (in the Schoenflies notation), and general x, y, and z coordinates (expressed as fractions of the lattice constants) for that site type, for each constituent of the host crystal

(f) Lattice constants a, b, and c (in Å) and angles $\alpha$, $\beta$, and $\gamma$ (in degrees and decimal parts)

(g) Effective charges (usually the valence charge) in units of the electronic charge

(h) Electric-dipole polarizabilities, $\alpha$ (in $Å^3$), for each of the constituent ions

### *2.2 Lattice sums, $A_{nm}$*

The data given in section 2.1 were used to obtain the point-charge,[2,3] point-dipole,[4] and self-induced[5] contributions to the lattice sum parameters $A_{nm}$. All the $A_{nm}$ for $1 \leq n \leq 5$ are given and are sufficient for the analysis of the $nd^N$ configuration. The units of $A_{nm}$ are $cm^{-1}/Å^n$. The crystal-field parameters for a particular ion are given by $B_{nm} = \langle r^n \rangle A_{nm}$, where $\langle r^n \rangle$ is the radial expectation value[6] of $r^n$ for the ion under consideration. At the bottom of each of the tables of $A_{nm}$ the lattice sums $S^{(0)}$, $S^{(2)}$, and $S^{(4)}$ are given.

The $S^{(0)}$ sum yields the interconfiguration shift[7] $\Delta E = \Delta E_0 - [\langle r^2 \rangle_{n'l'} - \langle r^2 \rangle_{nl}] S^{(0)}$, and the $S^{(k)}$ sums yield the Slater integral shifts as $\Delta F^{(2)} = -\langle r^2 \rangle^2 S^{(2)}$ and $\Delta F^{(4)} = -\langle r^4 \rangle^2 S^{(4)}$; the

[1] *International Tables for X-Ray Crystallography, I, Symmetry Groups, Eds., N. F. M. Henry and K. Lonsdale, Kynoch, Birmingham, U. K. (1969).*

[2] *C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Crystals, in Handbook on the Physics and Chemistry of Rare Earths, 5, K. Gschneidner and L. Erying, Eds., North-Holland, New York (1982).*

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[6] *S. Fraga, K. M. S. Saxena, and J. Karwowski, Handbook of Atomic Data, Elsevier, New York (1976).*

[7] *C. A. Morrison, Host Dependence of the Rare-Earth Ion Energy Separation $4f^N - 4f^{N-1}nl$, J. Chem. Phys., 2 (1980), 1001.*

units are such that if $\langle r^k \rangle$ is in Å units, then each shift is in units of $cm^{-1}$.

### 2.3 Experimental results

In this section we report all the experimental data in terms of the Slater integrals $F^{(k)}$ and the crystal-field parameters $B_{nm}$. Since a number of different notations exist, we describe in detail our conversion from each set of constants to $B_{nm}$ or $F^{(k)}$.

#### 2.3.1 Relation of Dq with $B_{40}$

In his article, McClure[8] gives the electric potential for a six-fold cubic array of charges at a distance R as

$$V = D(x^4 + y^4 + z^4 - 3/5\, r^4), \quad (1)$$

where $D = 35\, e/(4R^5)$. The potential energy, eV, can be written as

$$U = eDr^4(X^4 + Y^4 + Z^4 - 3/5), \quad (2)$$

where $X = x/r$, etc. For equivalent electrons, McClure[8] defines q by $q = 2\langle r^4 \rangle e/105$, so that

$$U = (105/2)Dq(X^4 + Y^4 + Z^4 - 3/5). \quad (3)$$

In our notation, we write the same potential as

$$U = B_{40}[C_{40} + (5/\sqrt{70})(C_{44} + C_{4-4})], \quad (4)$$

for six-fold cubic coordination with charges at $(\pm R,0,0)$, $(0,\pm R,0)$, and $(0,0,\pm R)$. The $C_{nm}$ are given by[9]

$$C_{40} = (35Z^4 - 30Z^2 + 3)/8, \quad (5)$$

$$C_{4\pm4} = (X \pm iY)^4(35/128)^{1/2}. \quad (6)$$

Substituting (5) and (6) into (4) gives

$$C_{40} + (5/\sqrt{70})(C_{44} + C_{4-4}) = (5/2)(X^4 + Y^4 + Z^4 - 3/5). \quad (7)$$

Thus, we obtain

$$(5/2)B_{40} = (105/2)Dq,$$

or

$$B_{40} = 21Dq. \quad (8)$$

This relation (8) has been used to convert the Dq reported in the literature to $B_{40}$ for crystals with four-fold axes (e.g., $C_4$, $S_4$, etc.). If in the cubic group the principal axis of rotation is the cube diagonal, then relation (4) becomes

$$U = B'_{40}[C_{40} + \sqrt{10}/\sqrt{7}(C_{43} - C_{4-3})], \quad (9)$$

and the reported Dq, $B_{40}$ relation becomes

$$B'_{40} = 14\, Dq \quad (10)$$

Since the sign of Dq is generally not reported, we give the sign of $B_{40}$ or $B'_{40}$ that is obtained from the point charge lattice sum $A_{40}$.

#### 2.3.2 Relation between Slater and Racah parameters

For d electrons, Judd[10] gives the following relations:

$$F_0 = F^{(0)}$$
$$F_2 = F^{(2)}/49$$
$$F_4 = F^{(4)}/441 \quad (11)$$

and

$$E^0 = F_0 - 7F_2/2 - 63F_4/2$$
$$E^1 = 5(F_2 + 9F_4)/2$$
$$E^2 = (F_2 - 5F_4)/2 \quad (12)$$

and Racah[11] introduces A, B, and C by

$$A = F_0 - 49F_4$$
$$B = F_2 - 5F_4$$
$$C = 35F_4 \quad (13)$$

[8] D. S. McClure, Electronic Spectra of Molecules and Ions in Crystals: II, Solid State Phys., 9 (1959), 420, Academic Press, New York.
[9] C. J. Ballhausen, Ligand Field Theory, McGraw Hill, New York (1962), 93.
[10] B. R. Judd, Operator Techniques in Atomic Spectroscopy, McGraw-Hill, New York (1963), 221.
[11] G. Racah, Theory of Complex Spectra IV, Phys. Rev., 76 (1949), 1352.

All these parameters are used and reported in the literature. We have chosen to put all the reported data in terms of $F^{(k)}$, since Hartree-Fock calculations of $F^{(k)}$ have been reported for a large number of ions.[6] In terms of A, B, and C we have

$$F^{(0)} = (5A + 7C)/5,$$

$$F^{(2)} = 7(7B + C),$$

and

$$F^{(4)} = 63C/5. \quad (14)$$

And in terms of $E^k$ :

$$F^{(0)} = E^0 - 49E^1/10 + 63E^2/2,$$

$$F^{(2)} = 49(9E^2 - E^1)/2,$$

and

$$F^{(4)} = 441(5E^2 - E^1)/10; \quad (15)$$

and the relation between $F^{(k)}$ and $F_k$ is given in equation (11).

*2.4 References for each host material*

The final section on each host material consists of a number of references to experimental and theoretical work that has been reported. This list, in most cases, is far from exhaustive and will be continuously updated as new work is reported or older references found. For a number of hosts, only x-ray data have been reported, and we have been unable to find any reference to optical data on transition elements in these hosts. On a number of host materials, references were found which contain important information on that host not contained in the tables. These references have been included.

## 3. SUMMARY

In this report we have provided the data on 12 host materials for lasers that use the transition metal ions. Included in each section are the crystallographic data, x-ray data, lattice sum parameters $A_{nm}$, crystal field parameters $B_{nm}$ (Dq), and spin-orbit constants ($\zeta$). One section includes the phenomenological free ion parameters $F^{(k)}$, $\zeta$, and $\alpha$, which have been obtained by fitting the reported free ion data. For each host, there is a bibliography which, dependent on that particular host, is more or less complete. We plan to update the data contained on each host material as well as on new host materials as additional information becomes available.

[6] *S. Fraga, K. M. S. Saxena, and J. Karwowski, Handbook of Atomic Data, Elsevier, New York (1976).*


## ACKNOWLEDGEMENTS

We thank Norman Brandt of the Harry Diamond Laboratories' library for his cooperation in responding to our many requests for special information searches and copies of numerous documents from obscure sources. Also, we wish to thank A. Linz, H. Jenssen, and B. Aull of the Massachusetts Institute of Technology for suggesting a number of the materials referenced here. Thanks also go to A. Pinto and J. Paul of the Night Vision and Electro-Optics Laboratory for suggested materials.


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(5) C. A. Morrison, G. F. de Sá, and R. P. Leavitt, *Self-Induced Multipole Contribution to the Single-Electron Crystal Field*, J. Chem. Phys., **76** (1982), 3899.

(6) S. Fraga, K. M. S. Saxena, and J. Karwowski, *Handbook of Atomic Data*, Elsevier, New York (1976).

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(9) C. J. Ballhausen, *Ligand Field Theory*, McGraw Hill, New York (1962), 93.

(10) B. R. Judd, *Operator Techniques in Atomic Spectroscopy*, McGraw-Hill, New York (1963), 221.

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## Table 1. $Y_3Al_5O_{12}$ (YAG)

**(A) Crystallographic data on $Y_3Al_5O_{12}$.**

**Cubic Ia3d, 230, Z = 8**

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| $Al_1$ | 16(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.0530 |
| $Al_2$ | 24(d) | $S_4$ | 3/4 | 0 | 1/4 | 3 | 0.0530 |
| Y | 24(c) | $D_2$ | 0 | 1/4 | 1/8 | 3 | 0.870 |
| O | 96(h) | $C_1$ | −0.0306 | 0.0512 | 0.1500 | −2 | 1.349 |

[a] *X-ray data, a = 12.000 Å, reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al ion in 24(d) ($S_4$) site in $Y_3Al_5O_{12}$.**

| $A_{nm}$ | Point charge | Self-induced | Dipole | Total |
|---|---|---|---|---|
| $A_{20}$ | 6,355 | −2,604 | 14,013 | 17,765 |
| $ReA_{32}$ | −27,522 | 8,609 | −11,957 | −30,870 |
| $ImA_{32}$ | 37,839 | −11,913 | 6,332 | 32,258 |
| $A_{40}$ | −25,089 | 11,879 | −8,516 | −21,726 |
| $ReA_{44}$ | −3,763 | 1,614 | 1,964 | −185.1 |
| $ImA_{44}$ | −9,108 | 4,740 | −2,875 | −7,243 |
| $ReA_{52}$ | −2,931 | 2,287 | −3,498 | −4,142 |
| $ImA_{52}$ | 4,328 | −3,207 | 3,640 | 4,762 |
| $\|A_{44}\|$ | 9,855 | — | — | 7,245 |

**(C) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al ion in 16(a) ($C_{3i}$) site in $Y_3Al_5O_{12}$ (rotated so that the z-axis is parallel to the (111) crystallographic axis).**

| $A_{nm}$ | Point charge | Self-induced | Dipole | Total |
|---|---|---|---|---|
| $A_{20}$ | 6,836 | −1,107 | −13,553 | −7,823 |
| $A_{40}$ | −20,054 | 8,166 | 3,273 | −8,615 |
| $ReA_{43}$ | 2,813 | −1,422 | 6,253 | 7,644 |
| $ImA_{43}$ | −22,370 | 8,639 | 2,348 | −11,383 |
| $\|A_{43}\|$ | 22,546 | — | — | 13,711 |

**(D) Experimental ($cm^{-1}$) values of $B_{40}$, $F^{(2)}$, and $F^{(4)}$ for $nd^N$ ions in $Y_3Al_5O_{12}$**

| Ion | $B_{40}$ | $F^{(2)}$ | $F^{(4)}$ | T | Site | Ref. | $nd^N$ |
|---|---|---|---|---|---|---|---|
| $Cr^{+3}$ | −23,730 | 53,438 | 34,978 | 300 | $C_{3i}$ | 3,16 | $3d^3$ |
| $Cr^{+3}$ | −23,072 | 55,806 | 36,806 | 300 | $C_{3i}$ | 4 | $3d^3$ |
| $Cr^{+3}$ | −24,150 | 53,760 | 40,320 | — | $C_{3i}$ | 10 | $3d^3$ |
| $Cr^{+3}$ | −23,380 | — | — | — | $C_{3i}$ | 6 | $3d^3$ |
| $Cr^{+3}$ | −22,960 | 54,600 | 40,950 | 77 | $C_{3i}$ | 11 | $3d^3$ |
| $Mn^{+3}$ | −27,650 | 59,500 | 32,130 | 300 | $C_{3i}$ | 3,10 | $3d^4$ |
| $Mn^{+4}$ | −27,874 | 53,540 | 43,456 | 300 | $C_{3i}$ | 4 | $3d^3$ |
| $Mn^{+4}$ | −44,100 | — | — | — | — | 5 | $3d^3$ |
| $Fe^{+3}$ | −26,950 | 39,690 | 15,876 | 300 | $C_{3i}$ | 3,10 | $3d^5$ |
| $Fe^{+3}$ | −17,682 | 49,224 | 36,477 | — | $C_{3i}$ | 5,8 | $3d^5$ |
| $Fe^{+3}$ | −21,756 | 51,023 | 42,979 | — | $S_4$ | 5,8 | $3d^5$ |
| $Co^{+3}$ | −25,200 | 56,630 | 34,020 | 300 | $C_{3i}$ | 3,10 | $3d^6$ |
| $Co^{+3}$ | −17,430 | — | — | — | $S_4$ | 12 | $3d^6$ |
| $Co^{+2}$ | −9,660 | — | — | — | $S_4$ | 12 | $3d^7$ |
| $Co^{+2}$ | −12,880 | — | — | — | $C_{3i}$ | 12 | $3d^7$ |
| $Ni^{+3}$ | −27,580 | 42,000 | 22,680 | 300 | $C_{3i}$ | 3,10 | $3d^7$ |
| $Rh^{+3}$ | −28,840 | 40,600 | 21,924 | — | $C_{3i}$ | 5 | $4d^6$ |
| $Pd^{+3}$ | −23,730 | 39,326 | 21,218 | — | $C_{3i}$ | 5 | $4d^7$ |
| $Pt^{+3}$ | −23,100 | 44,520 | 30,744 | — | $C_{3i}$ | 5 | $5d^7$ |
| $V^{+3}$ | −23,800 | — | — | — | $C_{3i}$ | 5 | $3d^2$ |
| $V^{+3}$ | −17,850 | — | — | — | $S_4$ | 5 | $3d^2$ |
| $V^{+4}$ | −30,800 | — | — | — | $C_{3i}$ | 5 | $3d^1$ |
| $V^{+4}$ | −26,250 | — | — | — | $S_4$ | 5 | $3d^1$ |

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**(B) Lattice sum data.**

**1. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site ($C_{3i}$) in the Pa3 form of $K_2NaAlF_6$.**

| $A_{nm}$ | Monopole | Dipole |
|---|---|---|
| $A_{20}$ | 20,464 | 4,881 |
| $A_{40}$ | −15,791 | −13,471 |
| $ReA_{43}$ | 14,510 | 12,897 |
| $ImA_{43}$ | 3,769 | 3,277 |

**2. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site ($O_h$) in the Fm3m form of $K_2NaAlF_6$.**

| $A_{nm}$ | Monopole | Dipole | Self-Induced | Total |
|---|---|---|---|---|
| $A_{40}$ | 23,267 | 15,593 | −12,274 | 26,586 |
| $A_{44}$ | 13,905 | 9,319 | −7,335 | 15,888 |

*$S^{(0)} = 16{,}750\ cm^{-1}/Å^2$*
*$S^{(2)} = 15{,}425\ cm^{-1}/Å^4$*
*$S^{(4)} = 2{,}551.3\ cm^{-1}/Å^8$*

## Table 2. $K_2NaAlF_6$

**(A) Crystallographic data on the two forms of $K_2NaAlF_6$.**

**1. Cubic Pa3, 205, Z = 4, elpasolite.**

| Ion | Site | Symm. | x[a] | y | z | q | α(Å$^3$)[b] |
|---|---|---|---|---|---|---|---|
| Na | 4(b) | $C_{3i}$ | 1/2 | 1/2 | 1/2 | 1 | 0.147 |
| K | 8(c) | $C_3$ | 1/4 | 1/4 | 1/4 | 1 | 0.827 |
| Al | 4(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.0530 |
| F | 24(d) | $C_1$ | 0.22 | 0.03 | 0.01 | −1 | 1.04 |

*[a] X-ray data, a = 8.11 Å, reference 1.*
*[b] Reference 2.*

**2. Cubic Fm3m, 225, Z = 4, elpasolite.**

| Ion | Site | Symm. | x[a] | y | z | q | α(Å$^3$)[b] |
|---|---|---|---|---|---|---|---|
| Al | 4(a) | $O_h$ | 0 | 0 | 0 | 3 | 0.0530 |
| Na | 4(b) | $O_h$ | 1/2 | 1/2 | 1/2 | 1 | 0.147 |
| K | 8(c) | $T_d$ | 1/4 | 1/4 | 1/4 | 1 | 0.827 |
| F | 24(e) | $C_{4v}$ | 0.219 | 0 | 0 | −1 | 1.04 |

*[a] X-ray data, a = 8.119 Å, reference 6.*
*[b] Reference 2.*

### Table 2 References


(1) R. W. G. Wyckoff, *Crystal Structures*, **3**, Interscience, New York (1968), 374.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) C. D. Adam, *ENDOR Determination of Covalency in $K_2NaAlF_6$, $Cr^{3+}$*, J. Phys. C: Solid State Phys. **14** (1981), L105.

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(5) K. Grjotheim, J. G. Holm, and S. A. Mikhaiel, *Equilibrium Studies in the Systems $K_3AlF_6$-$Na_3AlF_6$ and $K_3AlF_6$-$Rb_3AlF_6$*, Acta Chem. Scand. **27** (1973), 1299.

(6) L. R. Morss, *Crystal Structure of Dipotassium Sodium Fluoroaluminate (Elpasolite)*, J. Inorg. Nucl. Chem. **36** (1974), 3876.


## Table 3. $Na_3Al_2Li_3F_{12}$ Cryolithionite (Garnet)

**(A) Crystallographic data on $Na_3Al_2Li_3F_{12}$.**

**Cubic Ia3d, 230, Z = 8.**

| Ion | Site | Symm. | x[a] | y | z | q | α(Å$^3$)[b] |
|---|---|---|---|---|---|---|---|
| Na | 24(c) | $D_2$ | 1/8 | 0 | 1/4 | 1 | 0.179 |
| Al | 16(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.0530 |
| Li | 24(d) | $S_4$ | 3/8 | 0 | 1/4 | 1 | 0.0321 |
| F | 96(h) | $C_1$ | −0.02888 | 0.04268 | 0.13989 | −1 | 0.731 |

*[a] X-ray data, a = 12.122 Å, from reference 1.*
*[b] Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site ($C_{3i}$) in $Na_3Al_2Li_3F_{12}$ (rotated so that the z-axis is along the (111) crystallographic axis).**

| $A_{nm}$ | Monopole | Total |
|---|---|---|
| $A_{20}$ | −2,050.90 | 732.86 |
| $A_{40}$ | 14,469.88 | −15,454.32 |
| $A_{43}$ | −16,491.07 | 18,471.61 |

### Table 3 References


(1) R. W. G. Wyckoff, *Crystal Structures*, **3**, Interscience, New York (1968), 222.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.


## Table 4. Free ion data

**Free ion $F^{(2)}$, $F^{(4)}$, and $\zeta$ and $\alpha$ for $nd^N$ ions ($cm^{-1}$).**

| $nd^N$ | Ion | $F^{(2)}$ | $F^{(4)}$ | $\zeta$ | $\alpha$ | Ref. |
|---|---|---|---|---|---|---|
| $3d^2$ | $Sc^{1+}$ | 35,469 | 19,832 | 63.18 | 27 | 1 |
| $3d^2$ | $Ti^{2+}$ | 53,061 | 30,920 | 126.4 | 56.4 | 1 |
| $3d^2$ | $Ti^{2+}$ | 54,870 | 32,034 | 129.4 | 20.80 | 2 |
| $3d^2$ | $Ti^{2+}$ | 53,322[a] | 29,000[a] | 120.4[b] | — | 3 |
| $3d^2$ | $V^{3+}$ | 67,200 | 40,522 | 219.6 | 75 | 1 |
| $3d^2$ | $Cr^{4+}$ | 75,831 | 47,061 | 337.9 | — | 1 |
| $3d^3$ | $V^{2+}$ | 55,153 | 20,954 | 186.3 | 199 | 1 |
| $3d^3$ | $V^{2+}$ | 59,669 | 35,882 | 176.7 | 24.58 | 2 |
| $3d^3$ | $V^{2+}$ | 57,437[a] | 36,363[a] | 167.8[b] | — | 4 |
| $3d^3$ | $Cr^{3+}$ | 75,950 | 30,076 | 295.6 | 437 | 1 |
| $3d^3$ | $Cr^{3+}$ | 70,905[a] | 45,986[a] | 296.4[b] | — | 5 |
| $3d^3$ | $Mn^{4+}$ | 80,332 | 47,754 | 437.0 | 91 | 1 |
| $3d^4$ | $Cr^{2+}$ | 59,121[a] | 46,179[a] | 234.3[b] | — | 5 |
| $3d^4$ | $Cr^{2+}$ | 62,300 | 38,934 | 263.2 | 61.0 | 1 |
| $3d^4$ | $Cr^{2+}$ | 64,467 | 39,730 | 239.4 | 28.36 | 2 |
| $3d^4$ | $Mn^{3+}$ | 81,970 | 46,998 | 387.7 | 12 | 1 |
| $3d^4$ | $Mn^{3+}$ | 71,593[a] | 55,647[a] | 361.8[b] | — | 6 |
| $3d^4$ | $Fe^{4+}$ | 87,269 | 56,183 | 564.6 | 85 | 1 |
| $3d^5$ | $Mn^{2+}$ | 67,685 | 40,698 | 351.4 | 74.8 | 7 |
| $3d^5$ | $Mn^{2+}$ | 69,266 | 43,578 | 317.5 | 32.14 | 2 |
| $3d^6$ | $Fe^{2+}$ | 79,149 | 49,153 | 440.5 | 81 | 1 |
| $3d^6$ | $Fe^{2+}$ | 74,064 | 47,426 | 411.0 | 35.92 | 2 |
| $3d^6$ | $Co^{3+}$ | 84,377[a] | 60,291[a] | 584.6[b] | — | 8 |
| $3d^7$ | $Co^{2+}$ | 77,532 | 50,123 | 560.3 | 65 | 1 |
| $3d^7$ | $Co^{2+}$ | 78,863 | 51,274 | 519.9 | 39.70 | 2 |
| $3d^8$ | $Ni^{2+}$ | 86,933 | 60,871 | 701.7 | 42 | 1 |
| $3d^8$ | $Ni^{2+}$ | 83,661 | 55,122 | 644.2 | 43.48 | 2 |

*[a]The Slater parameters are obtained by fitting the centroids of the reported experimental data for a given $nd^N$ configuration.*
*[b]The $\zeta$ values are obtained by fitting the lowest J multiplet of the Hund ground state of the $nd^N$ configuration.*

### Table 4 References


(1) W.-K. Li, *Magnetic Interactions in Transition Metal Ions, Part I. Electronic Configurations $d^2$, $d^3$, and $d^4$*, Atomic Data **2** (1970), 45.
W.-K. Li, *Magnetic Interactions in Transition Metal Ions, Part II. Bivalent Cations of the First Transition Series*, Atomic Data **2** (1970), 58.

(2) A. Pasternak and Z. B. Goldschmidt, *Spin-Dependent Interactions in the $3d^N$ Configurations of the Third Spectra of the Iron Group*, Phys. Rev. **A6** (1972), 55.
The parameters are given in the form

$F^{(2)} = 69{,}266 + 4{,}798.5(N - 5)$

$F^{(4)} = 43{,}578 + 3{,}848(N - 5)$

$\alpha = 32.14 + 3.78(N - 5)$

$\zeta = 348.3 + 85.8(N - 5) + 7.7[(N - 5)^2 - 4]$

(3) C. Corliss and J. Sugar, *Energy Levels of Titanium, Ti I through Ti XXII*, J. Phys. Chem. Ref. Data **8** (1979), 1.

(4) J. Sugar and C. Corliss, *Energy Levels of Vanadium, V I through V XXIII*, J. Phys. Chem. Ref. Data **7** (1978), 1191.

(5) J. Sugar and C. Corliss, *Energy Levels of Chromium, Cr I through Cr XXIV*, J. Phys. Chem. Ref. Data **6** (1977), 317.

(6) C. Corliss and J. Sugar, *Energy Levels of Manganese, Mn I through Mn XXV*, J. Phys. Chem. Ref. Data **6** (1977), 1253.

(7) T. M. Dunn and W.-K. Li, *Magnetic Interactions for the Electronic Configuration $d^5$*, J. Chem. Phys. **46** (1967), 2907.

(8) J. Sugar and C. Corliss, *Energy Levels of Cobalt, Co I through Co XXVII*, J. Phys. Chem. Ref. Data **10** (1981), 1097.


## Table 5. $Cs_2TlF_6$

**(A) Crystallographic data (two forms reported) on $Cs_2TlF_6$.**

**1. Cubic Fm3m, 225, Z = 4.**

| Ion | Site | Symm. | x[a] | y | z | q | $\sigma(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| Ti | 4(a) | $O_h$ | 0 | 0 | 0 | +4 | 0.506 |
| Cs | 8(c) | $T_d$ | 1/4 | 1/4 | 1/4 | +1 | 2.492 |
| F | 24(e) | $C_{4v}$ | 0.195 | 0 | 0 | −1 | 0.731 |

*[a]X-ray data, a = 8.96 Å, the F position is not reported for $Cs_2TlF_6$ and is taken from $Cs_2MnF_6$, reference 1.*
*[b]Reference 3.*

**2. Hexagonal $P\bar{3}m1$, 164, Z = 1.**

| Ion | Pos. | Symm. | x[a] | y | z | q | $\sigma(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| Ti | 1(a) | $D_{3d}$ | 0 | 0 | 0 | +4 | 0.506 |
| Cs | 2(d) | $C_{3v}$ | 1/3 | 2/3 | 0.691 | +1 | 2.492 |
| F | 6(i) | $C_s$ | 0.167 | 0.167 | 0.206 | −1 | 0.731 |

*[a]X-ray data, a = 6.15 Å, c = 4.96 Å, the Cs and F positions are not reported for $Cs_2TlF_6$ and are taken from $Cs_2ZrF_6$, reference 2.*
*[b]Reference 3.*

(B) Lattice sums.

1. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Ti site ($O_h$) in the cubic form of $Cs_2TiF_6$.

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{40}$ | 25,400 | 32,148 | −14,102 | 43,445 |
| $A_{44}$ | 15,179 | 19,212 | −8,428 | 25,963 |

$S^{(0)} = 18,682\ cm^{-1}/Å^2$
$S^{(2)} = 17,743\ cm^{-1}/Å^4$
$S^{(4)} = 3,148.1\ cm^{-1}/Å^8$

2. Lattice sums, $A_{nm}(cm^{-1}/Å^n)$, for the Ti site ($D_{3d}$) in the hexagonal form of $Cs_2TiF_6$.

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{20}$ | −5,629 | −3,291 | 1,172 | −7,748 |
| $A_{40}$ | −5,090 | −3,546 | 1,986 | −6,651 |
| $A_{43}$ | 10,051 | 6,316 | −3,059 | 13,308 |

$S^{(0)} = 8,919\ 9\ cm^{-1}/Å^2$
$S^{(2)} = 5,251.8\ cm^{-1}/Å^4$
$S^{(4)} = 460.86\ cm^{-1}/Å^8$

### Table 5 References


(1) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 341.

(2) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 350.

(3) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(4) N. B. Manson, G. A. Shah, B. Howes, and C. D. Flint, $^4A_g \leftrightarrow {}^2E_g$ *Transition of* $Mn^{4+}$ *in* $Cs_2TiF_6{:}MnF_6^{2-}$, Molec. Phys. **34** (1977), 1157.


## Table 6. $NH_4Al(SO_4)_2$

(A) Crystallographic data on $NH_4Al(SO_4)_2$.

Trigonal P321, 150, Z = 1.

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| $NH_4$ | 1(a) | $D_3$ | 0 | 0 | 0 | 1 | 2.684 |
| Al | 1(b) | $D_3$ | 0 | 0 | 1/2 | 3 | 0.0530 |
| S | 2(d) | $C_3$ | 1/3 | 2/3 | 0.222 | 6 | 4.893 |
| $O_1$ | 2(d) | $C_3$ | 1/3 | 2/3 | 0.016 | −2 | 1.349 |
| $O_2$ | 6(g) | $C_2$ | 0.328 | 0.344 | 0.317 | −2 | 1.349 |

[a] *X-ray data, a = 4.724 Å, c = 8.225 Å, the positions for S, $O_1$, and $O_2$ in $NH_4Al(SO_4)_2$ are not given. Those listed above are for the same ions in $KAl(SO_4)_2$, reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site ($D_3$) in $NH_4Al(SO_4)_2$.

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{20}$ | 13,668 | −42,591 | −2,720.0 | −41,994.49 |
| $A_{33}$ | 10,708 | −17,390 | −1,961.9 | — |
| $A_{40}$ | −4,089.1 | 25,994 | 4,005.7 | 25,293.63 |
| $A_{43}$ | 8,105.7 | −36,041 | 840.80 | 3,661.09 |
| $A_{53}$ | 5,996.4 | −15,968 | −2,489.0 | — |

$S^{(0)} = 15,593\ cm^{-1}/Å^2$
$S^{(2)} = 7,176.6\ cm^{-1}/Å^4$
$S^{(4)} = 444.17\ cm^{-1}/Å^8$

(C) Experimental parameters.

| Ion | $F^{(2)}$ | $F^{(4)}$ | $\zeta$ | $\alpha$ | $B_{40}$ | Ref. |
|---|---|---|---|---|---|---|
| $Cr^{3+}$ | — | — | 186 | — | 38,156 | 3 |

### Table 6 References


(1) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 168.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) S. V. J. Lakshaman, B. C. Venkatareddy, and J. Lakshmanarao, *Crystal Field, Spin Orbit and Excitation Interactions in the Spectrum of Chromium-Doped Ammonium Aluminum Sulphate*, Physica **98B** (1979), 65.


## Table 7. $MgF_2$

(A) Crystallographic data on $MgF_2$.

Tetragonal $P4_2/mnm$, 136, Z = 2.

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| Mg | 2(a) | $D_{2h}$ | 0 | 0 | 0 | +2 | 0.0809 |
| F | 4(f) | $C_{2v}$ | 0.303 | 0.303 | 0 | −1 | 0.731 |

[a] *X-ray data, a = 4.623 Å, c = 3.052 Å, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Mg site ($D_{2h}$) of $MgF_2$.**

| $A_{nm}$ | Monopole | Dipole | *Self-induced* | Total |
|---|---|---|---|---|
| $A_{20}$ | −576.3 | 3,745 | −592.7 | 2,576 |
| $A_{22}$ | 2,447 | −1,807 | −327.8 | 312.6 |
| $A_{40}$ | −3,020 | −381.7 | 660.3 | −2,742 |
| $A_{42}$ | −10,015 | −212.2 | 3,965 | −6,262 |
| $A_{44}$ | 4,458 | −513.4 | −2,057 | 1,887 |

*$S^{(0)} = 8,871\ cm^{-1}/Å^2$*
*$S^{(2)} = 6,315\ cm^{-1}/Å^4$*
*$S^{(4)} = 656.0\ cm^{-1}/Å^8$*

### Table 7 References


(1) R. W. G. Wyckoff, *Crystal Structures*, **1**, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Optical Maser Oscillation from $Ni^{2+}$* in $MgF_2$ Involving Simultaneous Emission of Phonons, Phys. Rev. Lett. **11** (1963), 318.

(4) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Spontaneous and Stimulated Emission from $Co^{2+}$* Ions in $MgF_2$ and $ZnF_2$, Appl. Phys. Lett. **5** (1964), 21.

(5) L. F. Johnson and H. J. Guggenheim, *Phonon-Terminated Coherent Emission from $V^{2+}$* Ions in $MgF_2$, J. Appl. Phys. **38** (1964), 483.

(6) R. R. Sharma and S. Sundaram, *Transition Metal Ions in Crystals: A Refined Treatment and Deduction of Coulomb and Exchange Interaction Constants*, Solid State Commun. **33** (1979), 381.

(7) S. I. Yun, L. A. Kappers, and W. A. Sibley, *Enhancement of Impurity Ion Absorption due to Radiation-Produced Defects*, Phys. Rev. **B5** (1973), 773.

(8) W. A. Sibley, S. I. Yun, and L. N. Feuerhelin, *Radiation Defect and 3d Impurity Absorption in $MgF_2$ and $KMgF_3$ Crystals*, J. Phys. (Paris) **34** (1973), C9-503.

(9) L. F. Johnson, H. J. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(10) M. D. Sturge, F. R. Merritt, L. F. Johnson, H. J. Guggenheim, and J. P. Van der Ziel, *Optical and Microwave Studies of Divalent Vanadium in Octahedral Fluoride Coordination*, J. Chem. Phys. **54** (1971), 1405.


## Table 8. $MnF_2$

**(A) Crystallographic data on $MnF_2$.**

**Tetragonal $P4_2/mnm$, 136, Z = 2.**

| Ion | Site | Symm. | x[a] | y | z | q | a[b] |
|---|---|---|---|---|---|---|---|
| Mn | 2(a) | $D_{2h}$ | 0 | 0 | 0 | +2 | 0.122 |
| F | 4(f) | $C_{2v}$ | 0.305 | 0.305 | 0 | −1 | 0.731 |

[a] *X-ray data, a = 4.8734 Å, c = 3.3099 Å, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$ for the Mn site ($D_{2h}$) in $MnF_2$.**

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{20}$ | 901.5 | 1,815.67 | −459.22 | 2,258 |
| $A_{22}$ | 2638 | −847.40 | −300.87 | 1,490 |
| $A_{40}$ | −1670 | −125.49 | 266.58 | −1,529 |
| $A_{42}$ | −7263 | −61.74 | 2,376.30 | −4,948 |
| $A_{44}$ | 3218 | −222.98 | −1,239.99 | 1,755 |

*$S^{(0)} = 6,070\ cm^{-1}/Å^2$*
*$S^{(2)} = 3,813\ cm^{-1}/Å^4$*
*$S^{(4)} = 307.3\ cm^{-1}/Å^8$*

**(C) Experimental parameters.**

| Ion | $F^{(2)}$ | $F^{(4)}$ | $\zeta$ | $B_{40}$ | Ref. |
|---|---|---|---|---|---|
| $Co^{2+}$ | — | — | — | −17,220 | 6 |

### Table 8 References


(1) R. W. G. Wyckoff, *Crystal Structures*, **1**, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Optical Maser Oscillation from $Ni^{+2}$* in $MgF_2$ Involving Simultaneous Emission of Phonons, Phys. Rev. Lett. **11** (1963), 318.

(4) L. F. Johnson, H. J. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(5) Von Werner H. Baur, *Uber die Verfeinerung der Kristallstrukturbestimmung einieger Vertreter des Rutiltyps, II. Die Difluoride von Mn, Fe, Co, Ni, und Zn*, Acta. Cryst. **11** (1958), 488.

(6) L. F. Blunt, *Optical Absorption of Cobalt in Manganese Fluoride*, J. Chem. Phys. **44** (1966), 2317.

### Table 8 References (cont'd)

(7) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Exchange Splitting of the Ground State of $Ni^{2+}$ Ions in Antiferromagnetic $MnF_2$, $KMnF_3$, and $RbMnF_3$*, Phys. Rev. Lett. **17** (1966), 13.

## Table 9. $ZnF_2$

**(A) Crystallographic data on $ZnF_2$.**

**Tetragonal $P4_2/mnm$, 136, Z = 2.**

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| Zn | 2(a) | $D_{2h}$ | 0 | 0 | 0 | +2 | 0.676 |
| F | 4(f) | $C_{2v}$ | 0.303 | 0.303 | 0 | −1 | 0.731 |

[a] *X-ray data, a = 4.7034 Å, c = 3.1335 Å, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Zn site ($D_{2h}$) in $ZnF_2$.**

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{20}$ | −304.8 | 2,855 | −593.0 | 1,957 |
| $A_{22}$ | 2,659 | −1,379 | −346.0 | 934.0 |
| $A_{40}$ | −249.1 | −268.3 | 430.1 | −2,329 |
| $A_{42}$ | −9,011 | −135.5 | 3,350 | −5,796 |
| $A_{44}$ | −4,046 | −383.2 | 1,786 | −1,876 |

*$S^{(0)} = 8,214.0\ cm^{-1}/Å^2$*
*$S^{(2)} = 5,417.7\ cm^{-1}/Å^4$*
*$S^{(4)} = 508.50\ cm^{-1}/Å^8$*

### Table 9 References

(1) R. W. G. Wyckoff, *Crystal Structures*, 1, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

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## Table 10. MgO

**(A) Crystallographic data on MgO.**

**Cubic Fm3m, 225, Z = 4.**

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha(Å^3)$[b] |
|---|---|---|---|---|---|---|---|
| Mg | 4(a) | $O_h$ | 0 | 0 | 0 | +2 | 0.0809 |
| O | 4(b) | $O_h$ | 1/2 | 1/2 | 1/2 | −2 | 1.349 |

[a] *X-ray data, a = 4.2112, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Mg site ($O_h$) in MgO.**

| $A_{nm}$ | Monopole | Self-induced | Total |
|---|---|---|---|
| $A_{40}$ | 20,084 | −5,812 | 14,271 |
| $A_{44}$ | 12,002 | −3,474 | 8,528.8 |

*$S^{(0)} = 11,851\ cm^{-1}/Å^2$*
*$S^{(2)} = 7,523.7\ cm^{-1}/Å^4$*
*$S^{(4)} = 621.35\ cm^{-1}/Å^8$*

**(C) Experimental parameters.**

| Ion | $F^{(2)}$ | $F^{(4)}$ | $\alpha$ | $B_{40}$ | Ref. |
|---|---|---|---|---|---|
| $Cr^{3+}$ | 50,906 | 37,825 | 70 | 33,579 | 5 |
| $V^{2+}$ | 42,429 | 30,239 | 60 | 30,429 | 5 |
| $Cr^{2+}$ | — | — | — | 14,000 | 14 |
| $Ni^{2+}$ | — | — | — | 18,060 | 15[a] |
| $Ni^{2+}$ | — | — | — | −17,115 | 16 |

[a] *Refers to experimental optical data by A. G. Shenstone, J. Opt. Soc. Am. 44 (1954), 749.*

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## Table 11. $Be_3Al_2(SiO_3)_6$ (Beryl, Emerald)

**(A) Crystallographic data on $Be_3Al_2(SiO_3)_6$.**

**Hexagonal P6/mcc, 192, Z = 2.**

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha$(Å$^3$)[b] |
|---|---|---|---|---|---|---|---|
| Al | 4(c) | $D_3$ | 1/3 | 2/3 | 1/4 | +3 | 0.0530 |
| Be | 6(f) | $D_2$ | 1/4 | 0 | 1/4 | +2 | 0.0125 |
| Si | 12(i) | $C_s$ | 0.382 | 0.118 | 0 | +4 | 0.0165 |
| $O_1$ | 12(i) | $C_s$ | 0.294 | 0.242 | 0 | −2 | 1.349 |
| $O_2$ | 24(m) | $C_1$ | 0.499 | 0.143 | 0.138 | −2 | 1.349 |

[a] *X-ray data, a = 9.206 Å, c = 9.205 Å, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site ($D_3$) in $Be_3Al_2(SiO_3)_6$.**

| $A_{nm}$ | Monopole | Dipole | Self-induced | Total |
|---|---|---|---|---|
| $A_{20}$ | −16,578 | 13,630 | 1,289 | −1,659 |
| $A_{33}$ | −14,113 | −12,941 | 12,339 | −14,716 |
| $A_{40}$ | −16,436 | −23,937 | 6,117 | −34,257 |
| $A_{43}$ | 20,357 | 29,273 | −8,341 | 41,288 |
| $A_{53}$ | −14,004 | −13,056 | 11,543 | −15,516 |

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## Table 12. $Na_3Li_3Sc_2F_{12}$

**(A) Crystallographic data on $Na_3Li_3Sc_2F_{12}$.**

**Cubic Ia3d, 230, Z = 8.**

| Ion | Pos. | Symm. | x[a] | y | z | q | $\alpha$[b] |
|---|---|---|---|---|---|---|---|
| Sc | 16(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.540 |
| Na | 24(e) | $D_2$ | 1/4 | 1/8 | 0 | 1 | 0.147 |
| Li | 24(d) | $S_4$ | 1/4 | 3/8 | 0 | 1 | 0.0321 |
| F | 96(f) | $C_1$ | −0.0343 | 0.0499 | 0.1407 | −1 | 0.731 |

[a] *X-ray data, a = 12.607 Å, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Sc site ($C_{3i}$) in $Na_3Li_3Sc_2F_{12}$ (rotated so that the z axis is along the (111) crystallographic direction).**

| $A_{nm}$ | Monopole | Total |
|---|---|---|
| $A_{20}$ | −107.71 | −307.29 |
| $A_{40}$ | 10,176 | −11,064 |
| $A_{43}$ | −11,848 | 13,385 |

$S^{(0)} = 10{,}262\ cm^{-1}/Å^2$
$S^{(2)} = 7{,}978.8\ cm^{-1}/Å^4$
$S^{(4)} = 947.55\ cm^{-1}/Å^8$

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## Table 13. $Na_3Li_3In_2F_{12}$

**(A) Crystallographic data on $Na_3Li_3In_2F_{12}$.**

**Cubic Ia3d, 230, Z = 8.**

| Ion | Site | Symm. | x[a] | y | z | q | $\alpha^b$ |
|---|---|---|---|---|---|---|---|
| In | 16(a) | $C_{3i}$ | 0 | 0 | 0 | 3 | 0.574 |
| Na | 24(c) | $D_2$ | 1/4 | 1/8 | 0 | 1 | 0.179 |
| Li | 24(d) | $S_4$ | 1/4 | 3/8 | 0 | 1 | 0.0321 |
| F | 96(f) | $C_1$ | −0.0349 | 0.0507 | 0.1422 | −1 | 0.731 |

[a] *X-ray data, a = 12.693, from reference 1.*
[b] *Reference 2.*

**(B) Lattice sums, $A_{nm}(cm^{-1}/Å^n)$, for the In site ($C_{3i}$) in $Na_3Li_3In_2F_{12}$ (rotated so that the z axis is along the (111) crystallographic axis).**

| $A_{nm}$ | Monopole | Total |
|---|---|---|
| $A_{20}$ | −123.31 | −482.55 |
| $A_{40}$ | −9150.3 | −10,065 |
| $A_{43}$ | 10,803 | 12,202 |

$S^{(0)} = 9{,}228.1\ cm^{-1}/Å^2$
$S^{(2)} = 6{,}898.8\ cm^{-1}/Å^4$
$S^{(4)} = 760.65\ cm^{-1}/Å^8$

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